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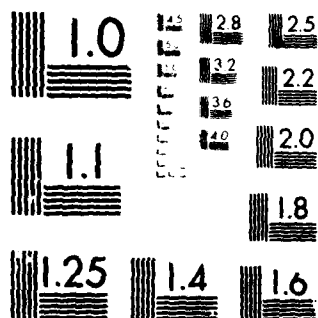


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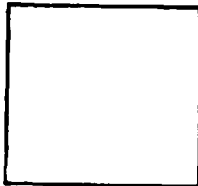


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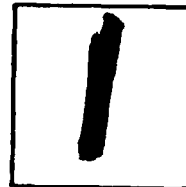
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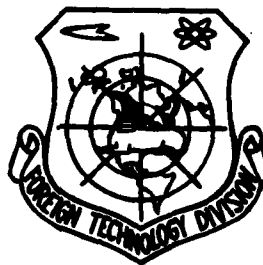
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ASSUMPTIONS IN ANALYZING THE SELF-IGNITION PROCESS OF
SHATTERED FUEL DROPS IN A HOT OXIDIZER

By

Piotr Wolanski



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ASSUMPTIONS IN ANALIZING THE SELF-IGNITION PROCESS OF SHATTERED FUEL DROPS IN A HOT OXIDIZER

Piotr Wolanski

The paper presents an analysis of a selection of assumptions in solving the mathematical model of self-ignition of shattered fuel drops in a hot oxidizer. A discussion is presented which concerns the criteria in selecting the values of the activation energy of chemical reactions and the necessity for considering heat balance for the evaporating drop is indicated. A critical attitude is taken toward accepting the assumption limiting the possibility of the appearance of chemical reactions beyond explosive limits. Doubt is also expressed on the possibility of using a model of self-ignition of a single drop to analyze the process of self-ignition of shattered drops in engine conditions.

The selection of assumptions with a mathematical model of the self-ignition process of fuel drops has an essential influence on the results of calculations obtained. With assumptions rather remote from reality the usability of obtained results can be debated, and for that reason particular attention should be given to the actual preciseness of the assumptions and the definition of the range of usefulness of the developed model.

This paper is a continuation of the discussion on this subject begun in (1). Some aspects of the discussion which stirred up controversy in the previous discussions (2), and which in an essential way influence the legitimacy of the model built are substantiated.

One of the notes concerned the identification of the possibility of the occurrence of chemical reactions with inflammability limits. After all, it is an evident fact that even one particle of fuel in the atmosphere of a hot gas oxidizer (and the reverse) over-reacts and gives off heat--although it does not create a flame. The quantity of fuel particles in the oxidizer (or the reverse) --their concentration--necessary to ^{produce} flames determines the limits of inflammability (or rather, explosiveness), and not the interval of appearance of chemical reactions. Thus if we leave a combustible mixture having an arbitrary composition in a vessel at a temperature lower than the self-ignition temperature, then it over-reacts without a flame appearing (the heat dispersed

is directed to the walls). Neglecting the possibility of chemical reactions in parts beyond the inflammability (explosive) limits can be only a simplification which in addition complicates the algorithm of calculations (through the introduction of additional conditions). In the case considered this has little bearing on the side of the over-enriched mixture, where the temperature is relatively low--thus the resulting speed of reaction is small. However in the area of lean mixtures where the temperature is sufficiently high and the reaction speed is relatively great the intervals can be larger. All things considered, a well-built mathematical model (in this aspect after eliminating simplified assumptions, it performs the task) determines, in which area and under what conditions an intensive (accelerated) chemical (flame) reaction can occur, and where and under what conditions the reaction is slow (no flame appears).

The occurrence of ignition (of an area of intense chemical reactions) at a specific distance from the surface of boiling liquid fuel results from the fact that in direct proximity to the fuel surface there is low temperature (intense cooling) and a low oxidizer concentration, which in effect does not lead to the existence of intense chemical reactions in this area. Thus the authors eliminated the erroneous corollary from the paper (3), of which I am coauthor and from the papers of other authors (4)-(6), in which the area of intense chemical reactions is recorded at a certain distance from the surface of the fuel.

It must be further understood, although this is not essential for a legitimate model, that the explosive (flammable) limits depend on the temperature of the combustible mixture (expand with an increase in temperature) (7), (8), while at a temperature higher than the temperature of self-ignition they do not have sense practically (8).

The next matter is the identification of the activation energy of the combustion reaction with the energy of the ignition activation. Can it be identified, under what conditions and to what extent?

The activation energy of ignition concerns the preliminary reactions occurring in the mixture to the time of its self-ignition, i. e. , in the period in which the temperature of the mixture does not change much, when after self-ignition has occurred (intense temperature increase) other reactions (another activation energy) dominate.

In the event of unfamiliarity with the kinetics of the chemical reactions of the tested mixture, a blended thermal mechanism of the reaction and resultant activation energy of chemical reactions is accepted to its mathematical description. For this purpose for homogeneous mixtures the activation energy of preliminary reactions, defined on the bases of an analysis of the characteristic of self-ignition delay from temperature, can be taken as the

activation energy. Theoretical (numerical) analysis shows that such an approximation gives small differences of these energies (to the order of about twelve percent), although practically, the values of these differences can be greater.

For heterogeneous mixtures these differences are considerably greater since in this case besides chemical reactions, other processes (e. g. , shattering of drops, evaporation and diffusion) influence the value of activation energy of ignition. This is seen after analyzing the dependence of self-ignition delay designated by the paper's authors for a drop of diethylcyclohexane in oxygen in a temperature function of Fig. 8 (9). If the authors wanted to define the activation energy of chemical reactions (which is in principle the activation energy of ignition) from the obtained dependence (as a result of their calculations) of the time of self-ignition delay, then it seems that it is one half smaller than the value of the activation energy of chemical reactions which they took to calculate. This is shown in Fig. 1, where for comparison, calculations are presented for a homogeneous combustible mixture.

The fact that at this time there is not sufficient data on the mechanism and activation energy of the oxidation of diethylcyclohexane in oxygen, does not justify placing an equals sign between the activation energy of ignition of a drop and the activation energy of chemical reactions of vapor of this fuel.

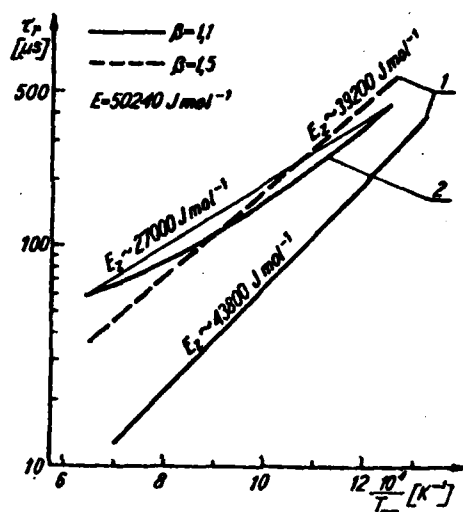


Fig. 1. Dependence of time of self-ignition delay on the temperature reciprocal is defined numerically. The given constants and coefficients taken for calculations are as in (9).

1--vapor mixture of diethylcyclohexane and oxygen with various values of coefficients of ignition criterium,

2--drops of diethylcyclohexane in oxygen (from ref. paper (9)).

The next matter concerns the magnitude of drops (microdrops) and consideration of evaporation in the mathematical model. Consideration in the mathematical model of the fact that the temperature at the border of the drop is always equal to the temperature of boiling fuel is not synonymous with a complete consideration of the evaporation process. This can only be true for large drops (not shattered) and small periods of self-ignition delay. In other instances consideration must also be made of the heat balance going to

the evaporation and the influence of evaporation on the change in magnitude (diameter) of the drop. This has particular significance in the case of the ignition of small drops or microdrops. Consideration of heat balance and the steaming mass of the drop would allow for the determination of the critical diameter of the drop, which can undergo self-ignition.

Besides fuel type, the following factors chiefly influence the size of the critical diameter of the drop: temperature of the gas medium and oxygen concentration. The critical diameter of the drop decreases with an increase of these parameters. The quantity of drops or limitation of shattering diffusing fuel vapors in the oxidizer also has an influence on the size of the critical diameter. With an increase in the quantity of drops their critical diameter decreases (10). Although for singular drops having a diameter smaller than critical self-ignition does not occur, in the case of an aerosol self-ignition can take place even after complete evaporation of a microdrop (the mixture of vapors of fuel and oxidizer ignites). In this aspect it would be meaningful to develop a model of microdrop self-ignition in a medium with a finite oxidizer excess (limited by areas occupied by successive microdrops). For such cases self-ignition can occur even after complete evaporation of a microdrop, but the so-called critical diameter of the drop has a different sense here.

In ignition of a "shattered" drop in the area of an aerosol we are dealing with a mixture of microdrops, their vapors and the gas oxidizer. This is a cause of their later explosive combustion. Using, for a mathematical description, this phenomenon of a model of the ignition of a single drop (not shattered) can not be a good approximation. In this aspect the mathematical model developed by the authors is not adequate for their physical model. This is one of the reasons that a good compatibility of the results of calculations with experimental tests was not achieved in a large range of changes in the concentration of oxygen in a gas oxidizer. The possibility of practical use of this model in engine testing is at least debatable, since for self-ignition of "shattered" drops in air the times of self-ignition delay calculated, based on the developed model differ with an order of magnitude from the times measured experimentally ($\tau_r \sim 300 \mu s$ from calculations, and $\tau_r \sim 3000 \mu s$ from measurements--Fig. 8 (9)).

Finally, I wish to note that the drawing of conclusions only from the comparison of equations used to describe various phenomena, without a penetrating analysis of the studies, should not be an argument in scientific discussion. This concerns the authors' assuming an attitude towards studies (3) and (11), of which I am a co-author. I wish to note that the mathematical models developed in these studies well approximate the achieved experimental results (12), (13) and that together with the co-author of these studies, they

sum up the situation well from the simplified assumptions (described in the studies) and from the scope of suitability of the models used.

Submitted
January, 1977

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